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Pseudogap and electrical properties in normal state cuprates

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Abstract : There are ample experimental evidences that suggest the existence of pseudogap around the Fermi level in normal state of high-T_c superconductor A possible mechanism based on removal of orbital degeneracy in Cu-O unit cell of cuprates has recently been proposed The density of states around the, Fermi level is obtained for different doping concentration and is found to be sensitive function of carrier concentration and next-nearest hopping The electrical conductivity has also been calculated. The resistivity changes metallic like to semiconductor like with onset of distortion in Cu-O cell associated with lifting of degeneracy. A peak appears at a characteristic temperature, which depends on electron-lattice interaction strength and carrier concentration.

Keywords High-T_c superconductor, pseudogap, cuprates

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1. Introduction

The existence of pseudogap that appears at certain temperature $T^* > T_c$ (superconducting transition temperature) in electronic spectra of high-T_c superconductor is considered to be the most important feature of the cuprates. The dip-like structure in the electronic density of states is referred to as pseudogap. Many experiments like NMR [1], angle-resolved photoemission spectroscopy (ARPES) [2], Specific heat [3], electron-tunneling spectroscopy (ETS) [4], scanning tunneling microscopy (STM) [5] have provided evidence in favour of such structure in electronic excitation spectra. The possible mechanisms like (i) a precursor pairing [6], (ii) a charge-density-wave gap [7], (iii) a spin gap due to antiferromagnetic correlation [8] have been considered earlier.

The structural transition from a tetragonal to an orthorhombic phase and the associated lowering of the symmetry has long been considered important in the high T_c superconductors. It has been recently proposed [9] that the structural distortion can lead to pseudogap behaviour in electronic density of states. In this communication, we present the results on density of states and electrical resistivity based on a simple model of cuprates.

2. Model and calculations

It is generally believed that the electrons in CuO_2 layer are mainly responsible for the unusual properties of the normal and superconducting states of high -T_c oxide materials. The electronic state of the CuO_2 layer is a combination of five states : one d-state of Cu and two p-states of each Oxygen. As p holes play a leading role in normal state transport and superconductivity, we consider only bonding p-states (p_x along x axis and p_y along y-axis in a layer) and neglect non-bonding orbitals.

In the undistorted phase, the electrons will 'see' the same site energy in 'a' and 'b' directions of the Cu-O layer, but the orthorhombic distortion will remove such degeneracy of site energy as the ligand field would shift the energy level differently in 'a' and 'b' directions of a unit cell (like Jahn-Teller distortion). This Jahn-Teller like distortion within the unit cell of the layer will lower the electronic energy. Moreover, the distortion will increase the elastic energy, which is proportional to the square of the distortion. So these two changes in energy compete with each other. For soft lattice, a distortion may result below at transition temperature.

We consider a model Hamiltonian [9] that describes the electronic motion in simplest form within the Cu-O layer.,

$$H = \sum \varepsilon_{p\alpha} p^{+}_{i\alpha\sigma} p_{i\alpha\sigma} + \sum t_{ij} \left(p^{+}_{i\alpha\sigma} p_{j\alpha'\sigma} + h.c \right)$$

$$+ \sum t'_{ij}\ p^{+}_{i\alpha\sigma} p_{j\alpha\sigma} \cdot \qquad (1)$$

Here, $\varepsilon_{p\alpha}$ represents site energy for the orbital α (where $p_x = 1$, $p_y = 2$) and for small distortion e, $\varepsilon_{p\alpha} = \varepsilon_0 \pm Ge$, G being the electron-lattice interaction constant. The compressed bond between Cu-O pushes up the energy level by Ge and elongation pushes down by same amount. The second term refers to the nearest neighbour hopping between p_x and p_y oxygen orbitals located at neigbouring sites i and j. The hopping along the same axis is mediated by Cu d-state and is represented by last term with t' as the next-nearest neighbour hopping integral (Figure 1). The Hamiltonian (1) can be written as

$$H = \sum_{k,\alpha} \varepsilon_{p\alpha} p^{+}_{k\alpha\sigma} p_{k\alpha\sigma} + \sum_{k,\alpha} \varepsilon_k p^{+}_{k\alpha\sigma} p_{k\alpha'\sigma}$$

where

$$\varepsilon_k = 4t \sin k_x a/2 \sin k_y a/2,$$

$$\varepsilon_{p\alpha} = 2t'(\cos k_x a + \cos k_y a) - \mu \pm Ge,$$

(+) for $\alpha = 1$, (−) for $\alpha = 2$.

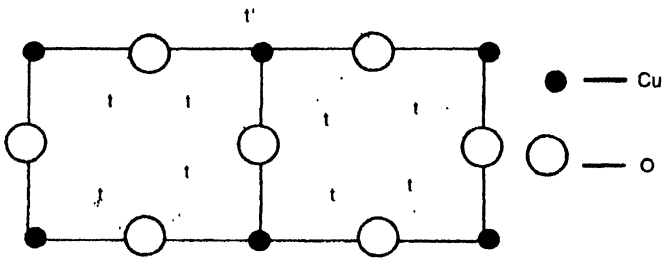

Figure 1.

We obtain energy dispersion and electron density of states by using Green's functions.

$$G_{\alpha\alpha'} = -\langle\langle p_{k\sigma\alpha}, p^{+}_{k\sigma\alpha'} \rangle\rangle,$$

$$G_{11}(\omega - \varepsilon_{p1}) = 1 + \varepsilon_k G_{21},$$

$$G_{21}(\omega - \varepsilon_{p2}) = \varepsilon_k G_{11}.$$

Here, $G_{\alpha\alpha'} = \sum_{k,i} \dfrac{A_{\alpha\alpha'}}{\omega - \omega_i} (i = +, -)$,

where $A_{\alpha\alpha'}$ is the spectral weight of the Green function, which is defined as

$$A_{\alpha\alpha} = \frac{\omega_+ - \varepsilon_{p\alpha}}{\Delta\omega} \delta(\omega - \omega_+) + \frac{\omega_- - \varepsilon_{p\alpha}}{\Delta\omega} \delta(\omega - \omega_-),$$

$$(\alpha = \alpha') \qquad (2)$$

$$A_{\alpha\alpha'} = \frac{\varepsilon_k}{\Delta\omega} \delta(\omega - \omega_+) - \frac{\varepsilon_k}{\Delta\omega} \delta(\omega - \omega_-),$$

α and α' take values 1 and 2.

The eigenvalues ω_i are

$$\omega_i = \omega_\pm = \frac{(\varepsilon_{p1} + \varepsilon_{p2}) \pm \sqrt{(\varepsilon_{p1} - \varepsilon_{p2})^2 + 4\varepsilon_k^2}}{2}$$

$$\Delta\omega = \omega_+ - \omega_-.$$

The density of states $\rho(\varepsilon)$ is easily obtained from the imaginary part of the Green function. The delta functions thus appear have been replaced by the Gaussian distribution with a broadening width τ for numerical simplification.

The corresponding free energy is

$$F = -kT \sum \ln\left[1 + e^{-\beta\omega_i}\right] + \frac{1}{2} Ce^2,$$

where $\frac{1}{2} Ce^2$ is the lattice strain energy with C the appropriate elastic constant.

The equilibrium value of the strain e is determined by minimizing the free energy. The equation for e becomes

$$1 = \frac{2G^2}{C} \sum_k \frac{\tanh(\beta\omega_+/2) - \tanh(\beta\omega_-/2)}{\omega_+ - \omega_-}. \qquad (3)$$

The chemical potential (μ) is determined by the number of electrons through the variation

$$n = \int \rho(\varepsilon) f(\varepsilon)\, d\varepsilon, \qquad (4)$$

where $f(\varepsilon)$ is the Fermi function. The solutions of e as a function of temperature and chemical potential were obtained numerically with the corresponding number density determined by the equation for n.

The temperature dependence of the gap or pseudogap and the DOS affect thermal variation of transport properties. The electrical conductivity is calculated from the current-current correlation function

$$\sigma_{xx} = \int \langle\langle j_x(\tau)\, j_x(0) \rangle\rangle\, d\tau,$$

where $j_x = -e \left[\sum_{k,\alpha} \dfrac{\delta\varepsilon_{p\alpha}}{\delta k_x} p^{+}_{\alpha k} p_{\alpha k} + \sum_{k,\alpha\neq\alpha'} \dfrac{\delta\varepsilon_k}{\delta k_x} p^{+}_{\alpha k} p_{\alpha' k} \right]$.

The conductivity can be recast in the form

$$\sigma = \int d\varepsilon \left(-\frac{\delta f}{\delta \varepsilon} \right) L(\varepsilon), \qquad (5)$$

where the function $L(\varepsilon)$ can be obtained from the Hamiltonian

$$L(\varepsilon) = e^2 \sum \left(\frac{\delta\varepsilon_{p\alpha}}{\delta k_y} \right)^2 + \left(\frac{\delta\varepsilon_k}{\delta k_x} \right)^2 \left[2A_{11}A_{22} + A_{12}^2 + A_{21}^2 \right],$$

where spectral weight A_{11}, A_{12} are obtained from the eq. (2).

3. Results and discussion

For numerical calculation, the value of the model parameters are chosen as t = 0.25 eV and the electron lattice deformation potential G^2/C = 0.18 eV. From eq. (3), it is apparent that the strain depends on parameter G^2/C, band structure and temperature. The variation of Δ = Ge (proportional to spontaneous strain) with temperature is displayed in Figure 2. The strain appears below a transition temperature T_p which depends sensitively on carrier concentration and G^2/C. The thermal variation of Δ is weak at $T < 0.5\ T_p$, and then sharply goes down to zero at T_p. The saturation value of strain also depends on the concentration and it is largest for the filling for which the Fermi level in undistorted phase is near the van Hove singularity. We note that it is important to consider the thermal shift of chemical potential for correct behaviour of Δ.

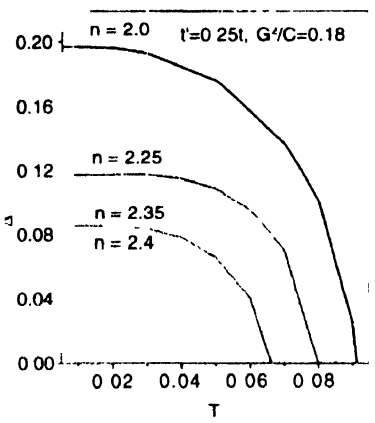

Figure 2. Strain (Δ) as a function of T for different concentration

The DOS in the undistorted state shows the 2D van Hove singularity whose position is a strong function of the relative values of t'/t. In our calculation we take the value of $t'/t = 0.25$. In Figure 3, we show the DOS for different values of temperature. At low temperature the gap appears around the Fermi level and it is due to spontaneous strain. With increase in temperature ($T > 0.5\ T_p$) the gap evolves in to a pseudogap defined by a dip in density of states. The pseudogap finally vanishes at T_p. The variation in DOS around the Fermi level is thus strong between $0.5T_p < T < T_p$. Thus the electronic properties like Knight shift,

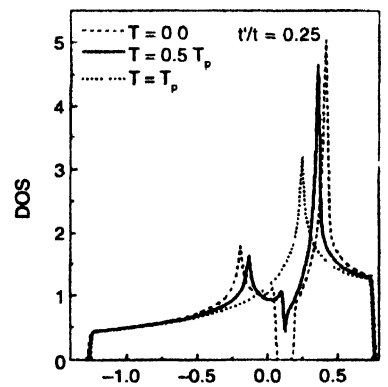

Figure 3. Distorted DOS *vs.* energy for different temperature.

Korringa relaxation time, specific heat *etc* that depends on DOS at Fermi level will have unusual behaviour. The electrical transport will be affected due to existence of pseudogap.

Figure 4 shows the resistivity (ρ) *vs* temperature for different electronic concentration. These concentrations are chosen so that the Fermi level in undistorted phase lies close to maximum of DOS. At high temperature $T > T_p$, ρ is metallic in nature and increases almost linearly with temperature. Resistivity changes from metallic to semiconductor like below T_p and passes through a peak as T is lowered. The peak value and its position depend on strain, which in turn depends on carrier concentration. For a real gap, the resistivity increases exponentially at low T. We note that it is assumed that adhoc electronic relaxation time τ is temperature independent.

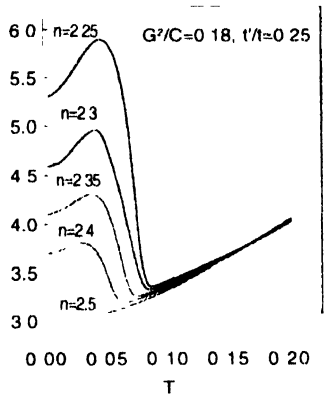

Figure 4. Resistivity *vs* temperature for different values of n

4. Conclusion

We consider a simple model for the structural distortion in cuprates where the degeneracy of oxygen p-level in Cu-O layer is removed by spontaneous distortion. This leads to opening a gap or pseudogap in DOS. In this process there is a net energy gain by the system by lowering its electronic energy over the increase in elastic energy. This gap or pseudogap strongly depends on the temperature and carrier concentration. In pseudogap region, the resistivity shows a typical metal to semiconductor transition with a peak below transition temperature. The electronic correlation effect which is ignored, will change the quantitative aspect of the results and will be treated in future.

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